

Connecting via Winsock to STN

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LOGINID:SSPTAVXR1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

***** Welcome to STN International *****

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NEWS 2 NOV 21 CAS patent coverage to include exemplified prophetic
substances identified in English-, French-, German-,
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NEWS 4 NOV 26 CHEMSAFE now available on STN Easy
NEWS 5 NOV 26 Two new SET commands increase convenience of STN
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NEWS 6 DEC 01 ChemPort single article sales feature unavailable
NEWS 7 DEC 12 GBFULL now offers single source for full-text
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NEWS 8 DEC 17 Fifty-one pharmaceutical ingredients added to PS
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NEWS 10 JAN 07 WPIDS, WPINDEX, and WPIX enhanced Japanese Patent
Classification Data

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

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agreement. Please note that this agreement limits use to scientific
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result in loss of user privileges and other penalties.

***** STN Columbus *****

FILE 'HOME' ENTERED AT 18:32:18 ON 27 JAN 2009

| | | |
|----------------------|------------|---------|
| => file registry | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.22 | 0.22 |

FILE 'REGISTRY' ENTERED AT 18:32:38 ON 27 JAN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 JAN 2009 HIGHEST RN 1096253-54-1
DICTIONARY FILE UPDATES: 26 JAN 2009 HIGHEST RN 1096253-54-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

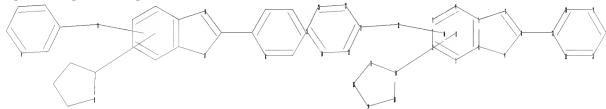
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10582564.str



chain nodes :

12

ring nodes :

1 2 3 4 5 6 7 8 9 10 13 17 18 19 20 21 22 23 24 25 26 27 28
29 30 31

chain bonds :

8-17 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-28 10-31 13-23 13-27 17-18
17-22 18-19 19-20 20-21 21-22 23-24 24-25 25-26 26-27 28-29 29-30 30-31

exact/norm bonds :

5-7 6-9 7-8 8-9 10-28 10-31 12-13 28-29 29-30 30-31

exact bonds :

8-17

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-23 13-27 17-18 17-22 18-19 19-20 20-21
21-22 23-24 24-25 25-26 26-27

G1:O,S

G2:Hy,Ph

Match level :

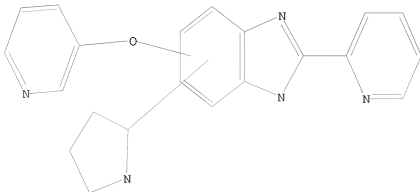
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:CLASS 13:Atom 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
 31:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S

G2 Hy,Ph

Structure attributes must be viewed using STN Express query preparation.

=> s sam sss l1

SAMPLE SEARCH INITIATED 18:33:13 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 64 TO ITERATE

100.0% PROCESSED 64 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 800 TO 1760

PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

=> d l2

L2 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN

RN 859538-93-5 REGISTRY

ED Entered STN: 11 Aug 2005

CN [1(2H),2'-Bipyridin]-2-one, 5'-[[2-(2-pyridinyl)-5-(2-pyrrolidinyl)-1H-benzimidazol-6-yl]oxy]- (CA INDEX NAME)

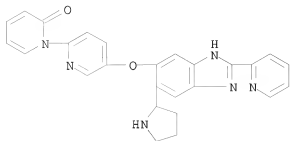
OTHER CA INDEX NAMES:

CN [1(2H),2'-Bipyridin]-2-one, 5'-[[2-(2-pyridinyl)-6-(2-pyrrolidinyl)-1H-benzimidazol-5-yl]oxy]- (9CI)

MF C26 H22 N6 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 12 2-8

L2 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN

RN 859535-88-9 REGISTRY

ED Entered STN: 11 Aug 2005

CN Ethanone, 1-[2-[6-[6-(difluoromethoxy)-3-pyridinyl]oxyl]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyrrolidine, 1-acetyl-2-[6-[6-(difluoromethoxy)-3-pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]- (9CI)

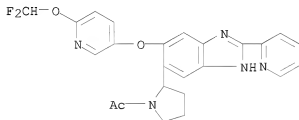
OTHER NAMES:

CN 6-(1-Acetylpyrrolidin-2-yl)-5-[[6-(difluoromethoxy)pyridin-3-yl]oxy]-2-(pyridin-2-yl)-1H-benzimidazole

MF C24 H21 F2 N5 O3

| SR | CA |
|----|----|
|----|----|

LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN

RN 859535-69-6 REGISTRY

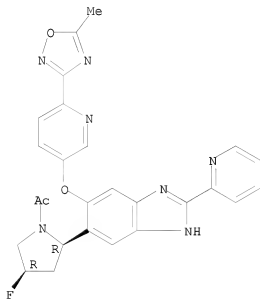
ED Entered STN: 11 Aug 2005

CN Ethanone, 1-[(2R,4R)-4-fluoro-2-[6-[[6-(5-methyl-1,2,4-oxadiazol-3-yl)-3-pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]-,

1. $\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$

rel- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Pyrrolidine, 1-acetyl-4-fluoro-2-[6-[[6-(5-methyl-1,2,4-oxadiazol-3-yl)-3-pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-, (2R,4R)-rel- (9CI)
 OTHER NAMES:
 CN cis-1-[4-Fluoro-2-[6-[[6-(5-methyl-1,2,4-oxadiazol-3-yl)pyridin-3-yl]oxy]-2-(pyridin-2-yl)-1H-benzimidazol-5-yl]pyrrolidin-1-yl]ethanone
 FS STEREOSEARCH
 MF C26 H22 F N7 O3
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

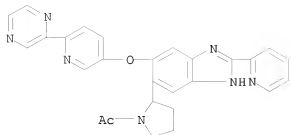
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 859535-56-1 REGISTRY
 ED Entered STN: 11 Aug 2005
 CN Ethanone, 1-[2-[6-[[6-(2-pyrazinyl)-3-pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]- (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Pyrrolidine, 1-acetyl-2-[6-[[6-(pyrazinyl)-3-pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]- (9CI)
 OTHER NAMES:
 CN 6-(1-Acetylpyrrolidin-2-yl)-5-[[6-(pyrazin-2-yl)pyridin-3-yl]oxy]-2-(pyridin-2-yl)-1H-benzimidazole
 MF C27 H23 N7 O2
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



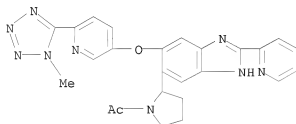
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```

L2 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN
RD 859535-32-3 REGISTRY
ED Entered STN: 11 Aug 2005
CN Ethanone, 1-[2-[6-[1-(1-methyl-1H-tetrazol-5-yl)-3-pyridinyl]oxy]-2-(2-
pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyrrolidine, 1-acetyl-2-[6-[1-(1-methyl-1H-tetrazol-5-yl)-3-
pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]- (9CI)
OTHER NAMES:
CN 6-(1-Acetylpyrrolidin-2-yl)-5-[[6-(1-methyl-1H-tetrazol-5-yl)pyridin-3-
yl]oxy]-2-(pyridin-2-yl)-1H-benzimidazole
MF C25 H23 N9 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

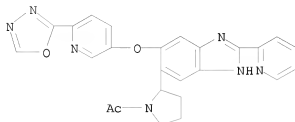
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```

LN      ANSWER 6 OF 8      REGISTRY    COPYRIGHT 2009 ACS on STN
RN      859534-96-6      REGISTRY
ED      Entered STN: 11 Aug 2005
CN      Ethanone, 1-[2-[6-[6-(1,3,4-oxadiazol-2-yl)-3-pyridinyl]oxyl]-2-(2-
        pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]- (CA INDEX NAME)
OTHER   CA INDEX NAMES:
CN      Pyrrolidine, 1-acetyl-2-[6-[6-(1,3,4-oxadiazol-2-yl)-3-pyridinyl]oxyl]-2-
        (2-pyridinyl)-1H-benzimidazol-5-yl]- (9CI)
OTHER   NAMES:
CN      6-(1-Acetylpyrrolidin-2-yl)-5-[6-(1,3,4-oxadiazol-2-yl)pyridin-3-yl]oxyl]-

```

2-(pyridin-2-yl)-1H-benzimidazole
 MF C25 H21 N7 O3
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN
 RN 859534-75-1 REGISTRY
 ED Entered SIN: 11 Aug 2005
 CN Ethanone, 1-[2-[6-([2,2'-bipyridin]-5-yloxy)-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyrrolidine, 1-acetyl-2-[6-([2,2'-bipyridin]-5-yloxy)-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-, mono(trifluoroacetate) (9CI)

OTHER NAMES:

CN 5-[[6-(1-Acetylpyrrolidin-2-yl)-2-(pyridin-2-yl)-1H-benzimidazol-5-yl]oxy]-2,2'-bipyridine monotrifluoroacetate

MF C28 H24 N6 O2 . C2 H F3 O2

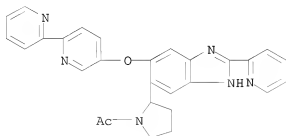
SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 859534-74-0

CMF C28 H24 N6 O2



CM 2

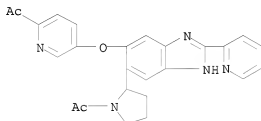
CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

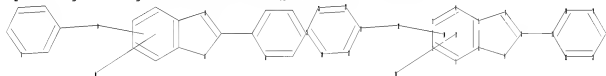
L2 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2009 ACS on STN
RN 859533-30-5 REGISTRY
ED Entered STN: 11 Aug 2005
CN Ethanone, 1-[2-[6-[(6-acetyl-3-pyridinyl)oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyrrolidine, 1-acetyl-2-[6-[(6-acetyl-3-pyridinyl)oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]- (9CI)
OTHER NAMES:
CN 1-[2-[6-[(6-Acetylpyridin-3-yl)oxy]-2-(pyridin-2-yl)-1H-benzimidazol-5-yl]pyrrolidin-1-yl]ethanone
MF C25 H23 N5 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>
Uploading C:\Program Files\STNEXP\Queries\10582564C.str



chain nodes :
10 12
ring nodes :
1 2 3 4 5 6 7 8 9 13 17 18 19 20 21 22 23 24 25 26 27


```

chain bonds :
8-17 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-23 13-27 17-18 17-22 18-19
19-20 20-21 21-22 23-24 24-25 25-26 26-27
exact/norm bonds :
5-7 6-9 7-8 8-9 12-13
exact bonds :
8-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-23 13-27 17-18 17-22 18-19 19-20 20-21
21-22 23-24 24-25 25-26 26-27

```

G1:O,S

G2:Hy,Ph

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:Atom 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom

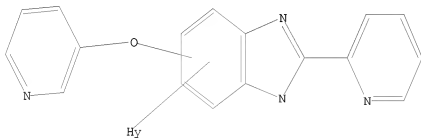
```

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR



G1 O,S

G2 Hy,Ph

Structure attributes must be viewed using STN Express query preparation.

=> s sam sss l3

SAMPLE SEARCH INITIATED 18:42:40 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 671 TO 1569

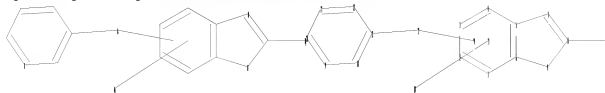
PROJECTED ANSWERS: 8 TO 329

L4

8 SEA SSS SAM L3

=>

Uploading C:\Program Files\STNEXP\Queries\10582564D.str



chain nodes :

10 12 17

ring nodes :

1 2 3 4 5 6 7 8 9 13 18 19 20 21 22

chain bonds :

8-17 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-18 13-22 18-19 19-20 20-21 21-22

exact/norm bonds :

5-7 6-9 7-8 8-9 8-17 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-18 13-22 18-19 19-20 20-21 21-22

G1:O,S

G2:Hy,Ph

Match level :

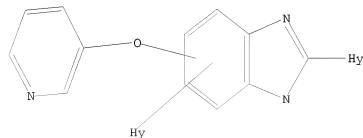
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:Atom 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom

L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



G1 O,S

G2 Hy,Ph

Structure attributes must be viewed using STN Express query preparation.

=> s 15 sss sam
SAMPLE SEARCH INITIATED 18:44:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1561 TO ITERATE

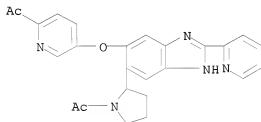
100.0% PROCESSED 1561 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 28850 TO 33590
PROJECTED ANSWERS: 9 TO 360

L6 9 SEA SSS SAM L5

=> d 16 9

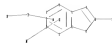
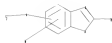
L6 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2009 ACS on STN
RN 859533-30-5 REGISTRY
ED Entered STN: 11 Aug 2005
CN Ethanone, 1-[2-[6-[(6-acetyl-3-pyridinyl)oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyrrolidine, 1-acetyl-2-[6-[(6-acetyl-3-pyridinyl)oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]- (9CI)
OTHER NAMES:
CN 1-[2-[6-[(6-Acetylpyridin-3-yl)oxy]-2-(pyridin-2-yl)-1H-benzimidazol-5-yl]pyrrolidin-1-yl]ethanone
MF C25 H23 N5 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=>
Uploading C:\Program Files\STNEXP\Queries\10582564B-1.str



```

chain nodes :
10 12 13 17
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
8-17 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 8-17 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

G1:O,S

G2:Hy,Ph

Match level :

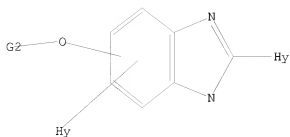
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:CLASS 13:Atom 14:Atom 17:Atom

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



G1 O,S

G2 Hy,Ph

Structure attributes must be viewed using SIN Express query preparation.

=> s l7 sam sss

SAMPLE SEARCH INITIATED 18:51:19 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 46545 TO ITERATE

4.3% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

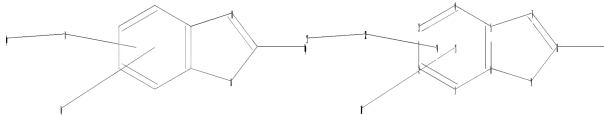
PROJECTED ITERATIONS: 918014 TO 943786

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=>

Uploading C:\Program Files\STNEXP\Queries\10582564F.str



chain nodes :

10 12 13 15

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

8-15 12-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9

exact/norm bonds :

5-7 6-9 7-8 8-9 8-15 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom

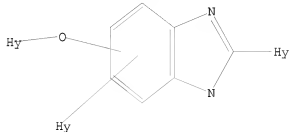
L9 STRUCTURE UPLOADED

=> d l9

L9 HAS NO ANSWERS

L9

STR



Structure attributes must be viewed using STN Express query preparation.

=> s sss sam l9

SAMPLE SEARCH INITIATED 18:57:10 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 50085 TO ITERATE

4.0% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 988338 TO 1015062

PROJECTED ANSWERS: 0 TO 0

L10

0 SEA SSS SAM L9

=> s l7 full sss

FULL SEARCH INITIATED 19:02:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 925193 TO ITERATE

100.0% PROCESSED 925193 ITERATIONS

117 ANSWERS

SEARCH TIME: 00.00.15

L11

117 SEA SSS FUL L7

=> d l11 1

L11 ANSWER 1 OF 117 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1034497-90-9 REGISTRY

ED Entered STN: 17 Jul 2008

CN Ethanone, 1-[(2R)-2-[6-[[6-(methoxymethyl)-3-pyridinyl]oxy]-2-(2-pyridinyl)-1H-benzimidazol-5-yl]-1-pyrrolidinyl]-, phosphate (1:1) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H25 N5 O3 . H3 O4 P

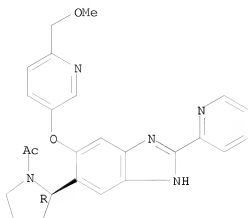
SR CA

LC STN Files: CA, CAPLUS, CASREACT

CM 1

CRN 1034497-89-6
CMF C25 H25 N5 O3

Absolute stereochemistry.



CM 2

CRN 7664-38-2
CMF H3 O4 P



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 231.34 | 231.56 |

FILE 'CAPLUS' ENTERED AT 19:04:22 ON 27 JAN 2009
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FILE COVERS 1907 - 27 Jan 2009 VOL 150 ISS 5

FILE LAST UPDATED: 26 Jan 2009 (20090126/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11

L12 4 L11

=> d l12 ibib abs 1-4

L12 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:643658 CAPLUS

DOCUMENT NUMBER: 149:104639

TITLE: Enantioselective Pd-Catalyzed α -Arylation of N-Boc-Pyrrolidine: The Key to an Efficient and Practical Synthesis of a Glucokinase Activator
AUTHOR(S): Klapars, Artis; Campos, Kevin R.; Waldman, Jacob H.; Zewge, Daniel; Dormer, Peter G.; Chen, Cheng-yi
CORPORATE SOURCE: Department of Process Research, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Journal of Organic Chemistry (2008), 73(13), 4986-4993
CODEN: JOCEAH; ISSN: 0022-3263

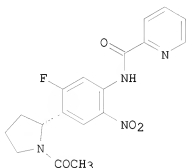
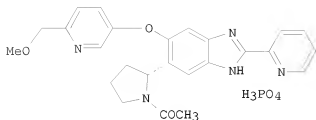
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:104639

GI



AB A short and practical synthesis of glucokinase activator I was achieved utilizing a convergent strategy involving SNAr coupling of activated aryl fluoride II with 3-hydroxy-6-(methoxymethyl)pyridine. The key to the success of the synthesis was the development of a novel method for enantioselective formation of α -arylpyrrolidines during the course of the project. In this method, (-)-sparteine-mediated enantioselective lithiation of N-Boc-pyrrolidine was followed by in situ transmetalation to zinc and Pd-catalyzed coupling with 2-fluoro-4-aminophenyl bromide, proceeding in 92% ee. This transformation allowed the preparation of compound

I in a 31% overall yield over six steps.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on SIN

ACCESSION NUMBER: 2007:110128 CAPLUS

DOCUMENT NUMBER: 146:206296

TITLE: Preparation of heterocyclylbenzimidazoles and their use as medical compositions, glucokinase inhibitors, antidiabetic agents, and antiobesity agents
Ogino, Yoshio; Nonoshita, Katsumasa; Nishimura, Teruyuki; Eiki, Junichi

INVENTOR(S): Banyu Pharmaceutical Co., Ltd., Japan

PATENT ASSIGNEE(S): Jpn. Kokai Tokkyo Koho, 93 pp.

SOURCE: CODEN: JKXXAF

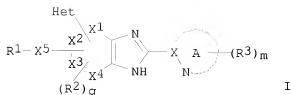
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| JP 2007022937 | A | 20070201 | JP 2005-204151 | 20050713 |
| PRIORITY APPLN. INFO.: | | | JP 2005-204151 | 20050713 |
| OTHER SOURCE(S): | MARPAT | 146:206296 | | |



AB Title compds. I [X, X1-X4 = C, N; ring A = 5- to 6-membered heteroaryl containing 1-4 N, S, and/or O; Het = 5- to 6-membered (un)substituted aliphatic heterocyclyl containing O or S; X5 = O, S, SO, SO2, SO2N, CO, NSO2; R1 = aryl, C1-6 alkyl, C3-7 cycloalkyl, (un)substituted (condensed) heteroaryl; R2 = CHO, OH, C1-6 alkyl, fluoromethyl(oxy), cyano, halo, etc.; R3 = C1-6 alkyl, (CH2)1-6OH, CO2-C1-6 alkyl, cyano, CO-C1-6 alkyl, halo, CO2H, etc.; R4 = (un)substituted C1-6 alkyl(oxy), C3-7 cycloalkyl, C2-6 alkenyl, (un)substituted amido, CO2-C1-6 alkyl, (un)substituted heterocyclyl, halo, CO2H, OH, NO2, etc.; m, q = 0-2] or their pharmacol. acceptable salts are prepared. Thus, cyclization of 5-carbaldehyde-6-[4-(ethylsulfonyl)phenoxy]-2-pyridin-2-yl-1H-benzimidazole with ethylene glycol gave dioxolane derivative, which inhibited human liver glucokinase with EC50 of 1.18 μ M.

L12 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2009 ACS ON SIN

ACCESSION NUMBER:

2007:61253 CAPLUS

DOCUMENT NUMBER:

146:142659

TITLE:

Preparation of heterocycle-substituted benzimidazole derivatives as glucokinase activators

INVENTOR(S):

Ogino, Yoshio; Nonoshita, Katsumasa; Nishimura, Teruyuki; Eiki, Jun-Ichi

PATENT ASSIGNEE(S):

Banyu Pharmaceutical Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 99pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|------------------|----------|
| WO 2007007910 | A1 | 20070118 | WO 2006-JP314307 | 20060712 |
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| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| AU 2006267338 | A1 | 20070118 | AU 2006-267338 | 20060712 |
| CA 2614544 | A1 | 20070118 | CA 2006-2614544 | 20060712 |
| EP 1905769 | A1 | 20080402 | EP 2006-781274 | 20060712 |
| R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, | | | | |

IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
 PRIORITY APPLN. INFO.: JP 2005-204438 A 20050713
 WO 2006-JP314307 W 20060712
 OTHER SOURCE(S): MARPAT 146:142659
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [X1-X4 = carbon or nitrogen atom; ring A = 5- to 6-membered heteroaryl having 1 to 4 heteroatoms independently selected from the group consisting of nitrogen, sulfur or oxygen atom; X = carbon or nitrogen atom; Het = 5- or 6-membered aliphatic heterocycle containing at least one nitrogen or sulfur atom and optionally addnl. heteroatom selected from the group consisting of nitrogen, sulfur or oxygen atom; wherein aliphatic heterocycle is optionally substituted with alkyl, -O-alkyl, oxo, etc.; X5 = -O-, -S-, -S(O)-, etc.; R1 = aryl, alkyl, cycloalkyl, etc.; R2 = formyl, -OH, alkyl, etc.; R3 = alkyl, -O-alkyl, cyano, etc.; m = 0-2; q = 0-2] and their pharmaceutically acceptable salts were prepared. For example, oxidation of [6-[4-(ethylsulfonyl)phenoxy]-2-pyridin-2-yl-1H-benzimidazol-5-yl]methanol, e.g., prepared from 2-fluoro-4-nitrobenzoic acid in 8 steps, using pyridine sulfur trioxide followed by reaction with ethylene glycol in the presence of p-TsOH.H2O afforded compound II. In glucokinase (GK) activation assays, the EC50 value of compound II was 1.18 μ M. Compds. I are claimed useful for the treatment of diabetes and obesity.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:612280 CAPLUS

DOCUMENT NUMBER: 143:153371

TITLE: Preparation of 2-heteroaryl-substituted benzimidazole derivatives as glucokinase activators

INVENTOR(S): Nonoshita, Katsumasa; Ogino, Yoshio; Ishikawa, Makoto; Sakai, Fumiko; Nakashima, Hiroshi; Nagae, Yoshikazu; Tsukahara, Daisuke; Arakawa, Keisuke; Nishimura, Teruyuki; Eiki, Junichi

PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 549 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

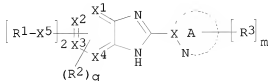
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|----------|
| WO 2005063738 | A1 | 20050714 | WO 2004-JP19843 | 20041228 |
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| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |

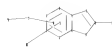
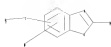
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| AU 2004309287 | A1 | 20050714 | AU 2004-309287 | 20041228 |
| AU 2004309287 | B2 | 20080731 | | |
| CA 2553160 | A1 | 20050714 | CA 2004-2553160 | 20041228 |
| EP 1702919 | A1 | 20060920 | EP 2004-808192 | 20041228 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | | |
| IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS | | | | |
| CN 1926127 | A | 20070307 | CN 2004-80042115 | 20041228 |
| BR 2004018212 | A | 20070427 | BR 2004-18212 | 20041228 |
| RU 2329261 | C2 | 20080720 | RU 2006-127420 | 20041228 |
| IN 2006DN03479 | A | 20070831 | IN 2006-DN3479 | 20060616 |
| MX 2006007462 | A | 20060809 | MX 2006-7462 | 20060628 |
| KR 2006105872 | A | 20061011 | KR 2006-713089 | 20060629 |
| NO 2006003475 | A | 20060928 | NO 2006-3475 | 20060728 |
| US 20080070928 | A1 | 20080320 | US 2007-582564 | 20070326 |
| PRIORITY APPLN. INFO.: | | | JP 2003-436992 | A 20031229 |
| | | | JP 2004-235696 | A 20040813 |
| | | | WO 2004-JP19843 | W 20041228 |
| OTHER SOURCE(S): MARPAT 143:153371 | | | | |
| GI | | | | |



AB The title compds. (I) [X, X1, X2, X3, X4 = C, N; ring A = a 5- or 6-membered nitrogenous aromatic heterocycle containing 1-3 heteroatoms selected from N, S, and O optionally fused to Ph or pyridyl; R1 = aryl, (un)substituted 4- to 10-membered monocyclic or bicyclic heterocyclyl containing 1-4 heteroatoms selected from N, S, and O; R2 = HO, CHO, CH3-aFa, OCH3-aFa, NH2, cyano, halo, C1-6 alkyl, (CH2)1-4-OH (wherein a = 1-3); R3 = C1-6 alkyl, (CH2)1-6-OH, CO2-C1-6 alkyl, (CH2)1-6-O-C1-6 alkyl, (CH2)1-6-NH2, cyano, CO-C1-6 alkyl, halo, C2-6 alkenyl, O-C1-6 alkyl, CO2H, OH, oxo; R4 = (un)substituted C1-6 alkyl, C3-7 cycloalkyl, C2-6 alkenyl, each (un)substituted CONH2, SO2NH2, O-C1-6 alkyl, or CO-C1-6 alkyl, etc.; X5 = O, S, S(O), SO2, single bond, O(CH2)1-6; q, m = 0-2] or pharmaceutically acceptable salts thereof are prepared. These compds. are glucokinase activators and useful as therapeutic and/or preventive agents for (1) diabetes, (2) complications of diabetes such as retinopathy, nephropathy, neurosis, ischemic heart disease, and arteriosclerosis, and (3) obesity. Thus, 0.026 mL pyridine-2-carboxaldehyde was added to a solution of 59 mg 3-(2-methoxyphenoxy)-5-(pyridin-3-yloxy)benzene-1,2-diamine in 0.5 mL nitrobenzene at 120° and stirred at the same temperature for 1 h to give 4-(2-methoxyphenoxy)-2-(pyridin-2-yl)-6-(pyridin-3-yloxy)-1H-benzimidazole (II). II in vitro activated 832 % human liver glucokinase expressed in Escherichia coli as flag fusion protein with EC50 of 1.4 μM.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
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ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 8-17 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

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G1:O,S

G2:Hy,Ph

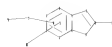
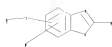
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11:Atom 12:CLASS 13:Atom 14:Atom 17:Atom

L13 STRUCTURE UPLOADED

=>

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chain nodes :
10 12 13 17
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
8-17 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 8-17 12-13
normalized bonds :
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G1:O,S

G2:Hy,Ph

Match level :

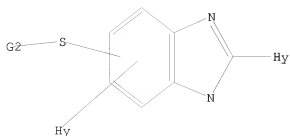
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11:Atom 12:CLASS 13:Atom 14:Atom 17:Atom

L14 STRUCTURE UPLOADED

=> d l14

L14 HAS NO ANSWERS

L14 STR



G1 O,S

G2 Hy,Ph

Structure attributes must be viewed using STN Express query preparation.

=> s sam sss l14

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 19:23:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 46545 TO ITERATE

4.3% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 918014 TO 943786

PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

L16 0 L15

=> s full sss l14

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 19:23:44 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 925193 TO ITERATE

100.0% PROCESSED 925193 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.15

L17 1 SEA SSS FUL L14

L18

1 L17

=> d 118

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:612280 CAPLUS

DN 143:153371

TI Preparation of 2-heteroaryl-substituted benzimidazole derivatives as glucokinase activators

IN Nonoshita, Katsumasa; Ogino, Yoshio; Ishikawa, Makoto; Sakai, Fumiko; Nakashima, Hiroshi; Nagae, Yoshikazu; Tsukahara, Daisuke; Arakawa, Keisuke; Nishimura, Teruyuki; Eiki, Junichi

PA Banyu Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 549 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|------------------|----------|
| PI | WO 2005063738 | A1 | 20050714 | WO 2004-JP19843 | 20041228 |
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| | RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | AU 2004309287 | A1 | 20050714 | AU 2004-309287 | 20041228 |
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| | CN 1926127 | A | 20070307 | CN 2004-80042115 | 20041228 |
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| | RU 2329261 | C2 | 20080720 | RU 2006-127420 | 20041228 |
| | IN 2006DN03479 | A | 20070831 | IN 2006-DN3479 | 20060616 |
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| | KR 2006105872 | A | 20061011 | KR 2006-713089 | 20060629 |
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| | US 20080070928 | A1 | 20080320 | US 2007-582564 | 20070326 |
| PRAI | JP 2003-436992 | A | 20031229 | | |
| | JP 2004-235696 | A | 20040813 | | |
| | WO 2004-JP19843 | W | 20041228 | | |

OS MARPAT 143:153371

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> exit

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS

| SINCE FILE ENTRY | TOTAL SESSION |
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| 2.75 | 449.17 |

FULL ESTIMATED COST

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|---------------------|------------------|
| CA SUBSCRIBER PRICE | 0.00 | -3.28 |

STN INTERNATIONAL LOGOFF AT 19:25:37 ON 27 JAN 2009